



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3HS9 / pdb_00003hs9
Title : Intersectin 1-peptide-AP2 beta ear complex
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Deposited on : 2009-06-10
Resolution : 2.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

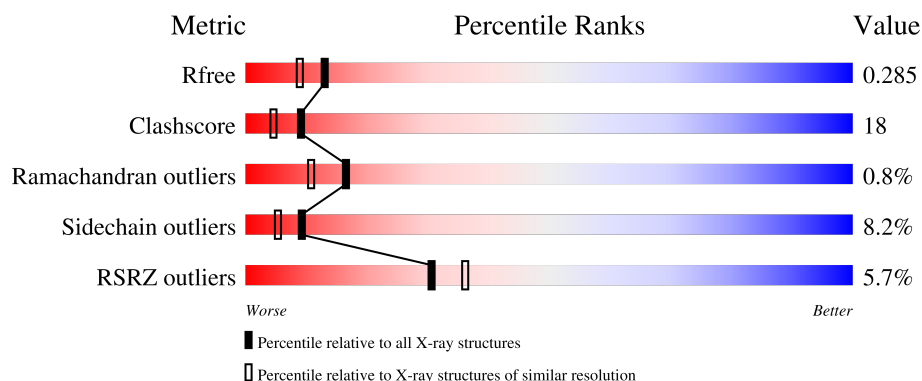
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	
2	P	12	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2085 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called AP-2 complex subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1858	1194	312	341	11			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	678	MET	-	expression tag	UNP P62944
A	679	GLY	-	expression tag	UNP P62944
A	680	SER	-	expression tag	UNP P62944
A	681	SER	-	expression tag	UNP P62944
A	682	HIS	-	expression tag	UNP P62944
A	683	HIS	-	expression tag	UNP P62944
A	684	HIS	-	expression tag	UNP P62944
A	685	HIS	-	expression tag	UNP P62944
A	686	HIS	-	expression tag	UNP P62944
A	687	HIS	-	expression tag	UNP P62944
A	688	SER	-	expression tag	UNP P62944
A	689	SER	-	expression tag	UNP P62944
A	690	GLY	-	expression tag	UNP P62944
A	691	LEU	-	expression tag	UNP P62944
A	692	VAL	-	expression tag	UNP P62944
A	693	PRO	-	expression tag	UNP P62944
A	694	ARG	-	expression tag	UNP P62944
A	695	GLY	-	expression tag	UNP P62944
A	696	SER	-	expression tag	UNP P62944
A	697	HIS	-	expression tag	UNP P62944
A	698	MET	-	expression tag	UNP P62944
A	699	ALA	-	expression tag	UNP P62944
A	700	SER	-	expression tag	UNP P62944

- Molecule 2 is a protein called peptide from Intersectin-1, residues 841-851.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	11	Total	C	N	O	0	0	0
			94	61	15	18			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	133	Total	O	0	0
			133	133		

- Molecule 1: AP-2 complex subunit beta-1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.09Å 47.10Å 58.95Å 90.00° 97.66° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 50.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-2.15) 95.7 (50.00-2.15)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.249 , 0.283 0.255 , 0.285	Depositor DCC
R_{free} test set	743 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.852	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2085	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.78	1/1901 (0.1%)	1.01	3/2583 (0.1%)
2	P	0.87	0/99	0.99	0/137
All	All	0.78	1/2000 (0.1%)	1.00	3/2720 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	854	ILE	CA-CB	5.22	1.59	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	782	ILE	N-CA-C	6.47	118.10	108.46
1	A	714	TRP	N-CA-C	-5.55	106.55	113.55
1	A	755	ILE	N-CA-C	5.10	116.05	108.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1858	0	1868	57	0
2	P	94	0	73	13	0
3	A	133	0	0	4	0
All	All	2085	0	1941	70	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 70 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:TYR:H	1:A:871:ASN:HD21	1.04	0.95
2:P:850:TRP:H	2:P:851:PRO:CD	1.80	0.92
1:A:751:THR:H	1:A:810:ASN:ND2	1.69	0.90
2:P:850:TRP:N	2:P:850:TRP:CD1	2.46	0.80
2:P:850:TRP:N	2:P:851:PRO:CD	2.47	0.74

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	231/260 (89%)	216 (94%)	14 (6%)	1 (0%)	30	27
2	P	9/12 (75%)	5 (56%)	3 (33%)	1 (11%)	0	0
All	All	240/272 (88%)	221 (92%)	17 (7%)	2 (1%)	16	11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	850	TRP
1	A	856	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/230 (91%)	192 (92%)	17 (8%)	9	5
2	P	10/11 (91%)	9 (90%)	1 (10%)	6	3
All	All	219/241 (91%)	201 (92%)	18 (8%)	9	5

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	922	GLU
2	P	848	SER
1	A	936	LYS
1	A	843	ASP
1	A	906	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	872	ASN
1	A	880	ASN
1	A	911	ASN
1	A	906	GLN
1	A	810	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	233/260 (89%)	0.52	11 (4%) 37 43	35, 50, 77, 85	0
2	P	11/12 (91%)	2.13	3 (27%) 2 2	20, 70, 72, 73	0
All	All	244/272 (89%)	0.59	14 (5%) 30 36	20, 51, 76, 85	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	851	PRO	8.0
2	P	849	THR	3.7
1	A	883	GLY	3.2
2	P	850	TRP	2.7
1	A	841	TRP	2.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.